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MODELING, SIMULATION, AND CONTROL OF AN EXTRATERRESTRIAL  
OXYGEN PRODUCTION PLANT

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### Abstract

The immediate objective of this project is the development of a new methodology for simulation of process plants used to produce oxygen and/or other useful materials from local planetary resources. Computer communication, artificial intelligence, smart sensors, and distributed control algorithms are being developed and implemented so that the simulation or an actual plant can be controlled from a remote location.

The ultimate result of this research will provide the capability for teleoperation of such process plants which may be located on Mars, Luna, an asteroid, or other objects in space [1,2]. A very useful near-term result will be the creation of an INTERACTIVE DESIGN TOOL, which can be used to create and optimize the process/plant design and the control strategy. This will also provide a vivid, graphic DEMONSTRATION MECHANISM to convey the results of other researchers to the sponsor.

### Introduction

In most areas of physical endeavor, the modern computer age has provided the possibility of performing design through modeling and simulation. The meta-laws in areas such as electrical or mechanical engineering are so well established that a plant (process) can be designed on the computer by use of well established modeling and simulation techniques before it is ever built. The design parameters identified in the simulation can then drive the process of implementation, and the resulting plant will, in all likelihood, function as anticipated by the simulation.

Chemical engineers and chemists are not at this stage of design yet. The area of chemical process modeling lags behind most other areas of physical system modeling. Meta-laws have been established, but they are valid only under specific (and often unstated) assumptions such as isothermal and isobaric, or isothermal and isochoric conditions. Furthermore, many of the necessary chemical process parameters have not been determined, and others are known with a very limited accuracy only. Therefore, it is essential that a chemical process design tool provides more than trajectory behavior only. It must be able to investigate the sensitivity of the design to inaccurately known parameter values. To solve these problems, we are utilizing a new methodology (bond graph modeling) which enables us to describe the complete dynamics of a chemical reaction

system and its environment.

In this project, we are working closely with Dr. Ramohalli to develop reasonable process flow diagrams for the testbed for his process for producing oxygen from carbon dioxide [3]. The dynamic parameters (the reaction rate constants) for the reaction kinetics equations that describe the reaction are being identified, as well as the static parameters of the energy equilibrium, such as the enthalpies of formation, the absolute entropies, and the heat capacitance functions of the materials involved. We are using our bond graph methodology to generate dynamic models of the processes, and we shall validate our models using experimental results from the testbed.

We are also creating a control model that allows us to optimally control the overall oxygen production plant, as well as an OASIS application data base and the data communication protocols that will allow us to teleoperate the locally controlled oxygen production plant [4,5]. This includes a preliminary investigation of the influence of smart components (smart sensors and smart controllers) on the degree of autonomy under which the plant can be operated, and a plan for future incorporation of artificial intelligence for increased autonomy.

Progress in the areas of modeling, communication, instrumentation and control, and artificial intelligence is described in the following sections.

### Modeling

A test bed system for extracting oxygen from carbon-dioxide (of which Mars' atmosphere is about 95%) has been designed and constructed at the University of Arizona - NASA Space Engineering Research Center, and is described elsewhere in this report. Development of simulation models of this test bed system is currently underway.

Three simulation models of the oxygen production system are of particular interest. The first involves the static mass flow of CO<sub>2</sub>, CO and O<sub>2</sub> within the system, and is based on thermodynamic and conservation of mass principles. From this simulation we can estimate what the production rate of oxygen will be in steady-state, and what various system pressures and temperatures can be expected to be.

The second simulation concerns the static energy flow within the system, and is based on thermodynamic and conservation of energy principles. This simulation allows conditions that were assumed in the first model to be verified, and enables an estimate to be made of the power requirements of the different system components.

The third simulation model will describe the dynamics of the system, and will be based on a modeling and design methodology involving the use of bond graphs. Bond graphs were originally introduced to model mechanical systems, and have since been adapted by Dr. Francois Cellier to model chemical reaction systems. Chemical reaction bond graphs model dynamic chemical reactions through the use of six variables; chemical potential, molar flow, hydraulic/pneumatic

pressure, volume flow, temperature and entropy flow. This will enable temperature and energy to be balanced for each separate subsystem of the entire system. These modular subsystems can then be connected together to form the model for the entire oxygen production plant, and valuable information can be learned about system start up and shut down, and optimal control strategies can be studied both for normal operation as well as for handling emergency situations.

The subsystem which performs the actual separation of the carbon dioxide into oxygen and carbon-monoxide is a zirconia cell. A dynamic model for this cell will be developed based on the chemical reaction and power balance which takes place within the cell. Separate program modules will be developed for each of the system processes, and then the simulation software DYMOLA will be used with DESIRE or ACSL to obtain a hierarchical coupling of these processes. The static simulation models are written in Ada and are currently running on a MicroVAX workstation at the University of Arizona. A remote controlling computer (another MicroVAX) sends input data to the local simulation computer over an Ethernet connection. The simulation executes on the local computer and then sends its results back to be displayed. The local simulation computer will eventually be moved out to the NASA center, which is several miles away from the University. Communication between the local and remote computers will then take place via a microwave link.

As the simulations and actual construction of the oxygen production plant enter their mature stages, model validation will be accomplished and the simulations will be used to give insight into which system configuration will result in optimum performance.

#### Communication

OASIS (Operations and Science Instrument System) is a software package developed by the University of Colorado in 1987. The purpose of OASIS is to allow remote operation of scientific experiments or remote supervisory control of telerobots or automated process plants. With this software, a remote commanding computer (RCC) on Earth would communicate with a local controlling computer (LCC) at some other location (e.g. Mars), which would implement the appropriate local control and monitoring algorithms [1, 2].

An OASIS application has been created to interact with the static mass flow model of the MARS test bed. The implementation of this application uses a MicroVAX II/GPX workstation (node name CACTUS) as the RCC and a second MicroVAX II/GPX workstation (node name PUEBLO) as the LCC. CACTUS prompts the user to enter certain information about the test bed (the flowrate of CO<sub>2</sub> into the system, the efficiency of the ZrO<sub>2</sub> cell, and the efficiency of the membrane separator). These data are sent to PUEBLO, where the temperatures, pressures and other mass flow rates of the system are calculated. The calculated values are transmitted back to CACTUS, where they are displayed for the user. The communication protocol presently employed is DECnet over an ethernet link within the same building. The protocol is currently being changed to TCP/IP,

and it will soon be tested over a microwave radio link to the testbed location which is about seven miles away.

Future work will include interfaces with the dynamic simulation and with the testbed itself, as illustrated in Figure 1. An expansion to allow multiple remote observers in addition to the remote commander will also be implemented, as well as a token passing protocol to allow any one of the observers to assume command.

#### Instrumentation and Control

An intelligent controller (smart sensor) which supports a fast local control loop has been used for control of a small testbed which was constructed for investigation of the seals between a section of stainless steel pipe and the zirconia cell. This controller has some simple programmable functions, limited logic functions and scaling capability for each instrumentation channel. It includes thermocouple transducers, a connection card, analog voltage input signal cards (for pressure transducers and flow meters), and a digital output signal card. The controller communicates commands and data with a 386 class personal computer (serving as the LCC) so that it can control a heater according to input commands from the computer.

More recently, the seven transducers of the oxygen production testbed have been connected to the smart sensor. Three thermocouple transducers are sensing temperatures of the input pipe, the  $ZrO_2$  cell pipe, and the output pipe. Two flow-meters and two pressure transducers are also used for monitoring the input and output gas streams. All these data are transferred to the LCC and the higher level control systems will generate appropriate control commands. Details of the high level control strategy are currently under development.

#### Artificial Intelligence

Some preliminary work has been initiated on a diagnostic system and related high autonomy concepts. The diagnostic system can be divided into two subsystems, the local diagnoser and the global diagnoser. The local diagnoser has shallow behavior knowledge of each component, and it will monitor the behavior discrepancies between its model and the real system. If there is any anomaly in readings from a sensor, for example, this will be detected by the local diagnoser, which will activate the global diagnoser to start a fault determination procedure. The fault will then be corrected locally, or further guidance will be requested from the remote commander.

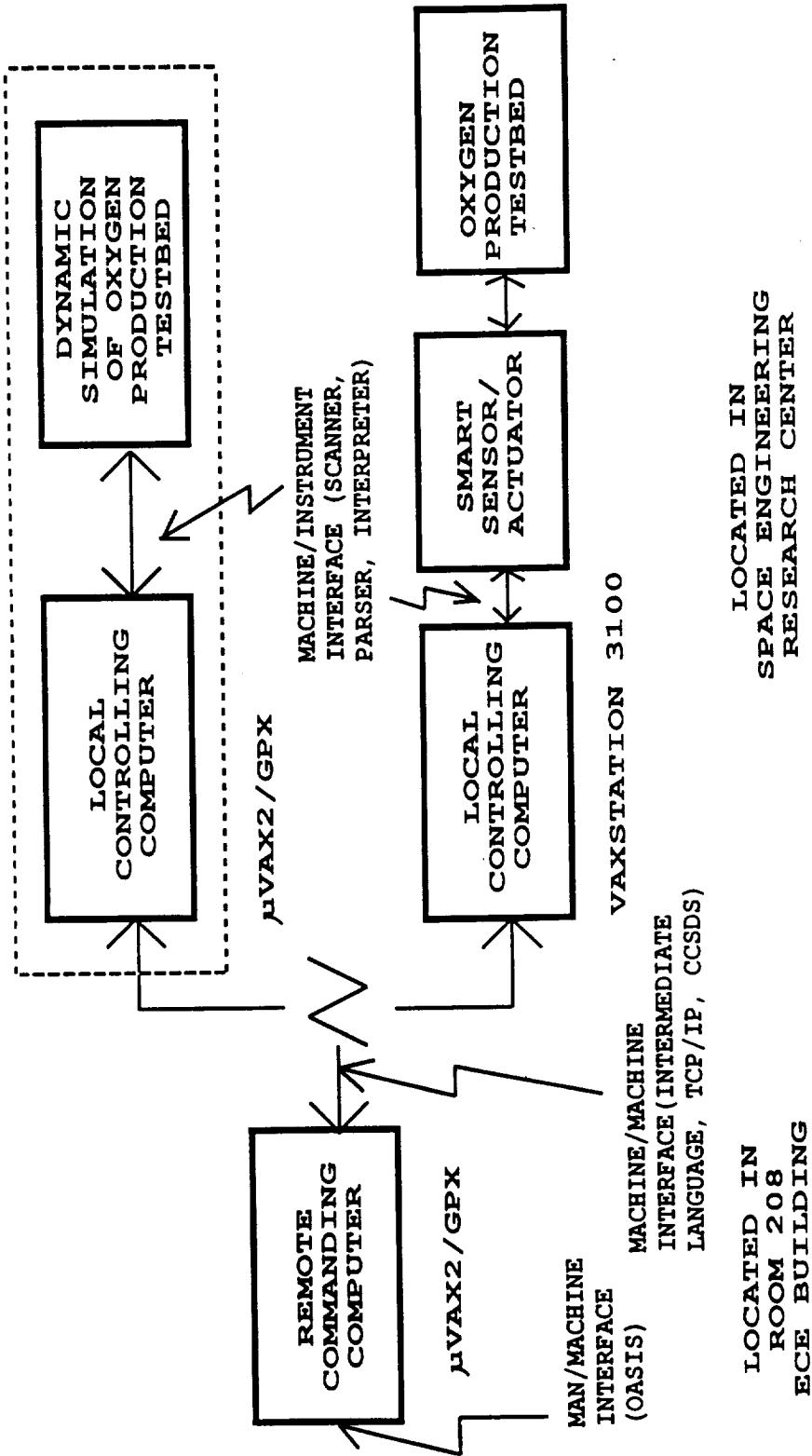
The local fault diagnoser models have been completed for the oxygen production portion, which includes the compressor, heat exchanger, temperature mixer, heater, temperature controller, and  $ZrO_2$  cell. Each component has its own causal effect model, which consists of shallow knowledge about the component, and it allows an experienced user to easily model the whole fault causal structure in a hierarchical manner. Each causal effect model is a rule



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Figure 1.  
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based model, and each fault event is associated with one or more rules. The inference of each fault event is different depending on the operational status of the component.

The global diagnoser simulator will run those fault diagnoser models and traverse all the possible causes that effect the fault symptom. The corresponding trajectories of event time for those causes will be generated as output from the simulator. Those trajectories can be used with the history records of sensors just before the anomaly is detected to determine the exact causes. Further development and implementation of these concepts will be proposed for the next contract period.

### Summary

All work on this project is proceeding on schedule. It is anticipated that the dynamic simulation will be completed, and that the dynamic simulation and/or the testbed will be capable of remote supervisory control by the end of the current contract period. Implementation of the higher level automation and control functions will be proposed for the next period.

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## **V. DATABASE DEVELOPMENT**